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J.-C. Fernandez-Toledano, T.D. Blake, P. Lambert, J. De Coninck

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On the cohesion of fluids and their adhesion to solids: Young's equation at the atomic scale

J-C. Fernandez-Toledano[a1], T. D. Blake[a], P. Lambert[b], and J. De Coninck[a]

[a] *Laboratory of Surface and Interfacial Physics (LPSI),University of Mons,7000 Mons, Belgium*

[b] *Université libre de Bruxelles - BEAMS CP165/56 - Av. F.D. Roosevelt 50 - B1050 Bruxelles*

Abstract

Using large-scale molecular dynamics simulations, we model a 9.2 nm liquid bridge between two solid plates having a regular hexagonal lattice and analyse the forces acting at the various interfaces for a range of liquid-solid interactions. Our objective is to study the mechanical equilibrium of the system, especially that at the three-phase contact line. We confirm previous MD studies that have shown that the internal pressure inside the liquid is given precisely by the Laplace contribution and that the solid exerts a global force at the contact line in agreement with Young's equation, validating it down to the nanometre scale, which we quantify. In addition, we confirm that the force exerted by the liquid on the solid has the expected *normal* component equal to $\gamma_{lv}\sin\theta^0$, where γ_{lv} is the surface tension of the liquid and θ^0 is the equilibrium contact angle measured on the scale of the meniscus. Recent thermodynamic arguments predict that the *tangential* force exerted by the liquid on the solid should be equal to the work of adhesion expressed as $Wa^0 = \gamma_{lv}(1+\cos\theta^0)$. However, we find that this is true only when any layering of the liquid molecules close to liquid-solid interface is negligible. The force significantly exceeds this value when strong layering is present.

Keywords: Wetting, adhesion, three-phase contact zone, liquid-solid interface, molecular-dynamics

Contents

[1] Corresponding author